

CONTENTS

ORIGINAL SCIENTIFIC PAPERS

Physical and Theoretical Chemistry

- M. J. Rioseras-Garcia and J. M. Hernando-Huelmo:** Theoretical Study of the Effect Exerted on the Periphery of 10-Anulene by Two Benzenoid Rings 1
- Y. I. Tur'yan:** Studying Kinetics of the Dehydration Reaction of Pyruvic Acid and Ethyl Pyruvate Using the Polarographic Kinetic Currents 13
- E. M. Rus, D. M. Constantin, L. Oniciu, and L. Ghergari:** Structural and Electrochemical Characteristics of Sintered Nickel Electrodes 25
- B. Kovač, L. Klasinc, E. Vukoša, L. Lončar-Tomašković, and M. Mintas:** HeI Photoelectron Spectra of *o,o'*-Bridged Biphenyls by 2-X-Propylene (X = O, S, SO, NCH₃) Chains 43
- M. Višić, R. Tomaš, and I. Mekjavić:** Stability Constants of Chlorocadmium Complexes in *t*-Butanol + Water Mixtures (*w*_{*t*BuOH} = 10%, 30%, and 50%) from Electromotive Force Measurements 55
- B. S. Andonovski:** UV Study of Protonation of Indole-2-Carboxylic Acid, 3-Methylindole, and D-Tryptophan in Perchloric Acid Solutions 711
- N. Raos:** Iterative Method for Finding the Low-Energy Conformations Based on the Model of Overlapping Spheres: Application to Alkanes 727
- D. Marijan, M. Vuković, P. Pervan, and M. Milun:** Surface Modification of Stainless Steel-304 Electrode. 1. Voltammetric, Rotating Ring-Disc Electrode and XPS Studies 737
- D. Marijan, R. Slavković, and M. Vuković:** Surface Modification of Stainless Steel-304 Electrode. 2. An Experimental Comparative Study of Electrochemically, Hydrothermally and Chemically Modified Oxide Films 751

T	T. Frentiu, S. D. Anghel, M. Nicola, E. Darvasi, A. Simon, and E. Cordos: Figures of Merit and Fundamental Processes in Analysis of Ca from Liquid Samples Using an r.f. CCP Torch with Tubular and Ring Electrodes	763
M. V. Diudea: Valencies of Properties	835	
A. Graovac, M. Juvan, B. Mohar, and J. Žerovnik: Computing the Determinant and the Algebraic Structure Count in Polygraphs	853	
A. A. Dobrynin: Explicite Relation between the Wiener Index and the Schultz Index of Catacondensed Benzenoid Graphs	869	
B. Grgas, S. Nikolić, N. Paulić, and N. Raos: Estimation of Stability of Copper(II) Chelates with <i>N</i> -Alkylated Amino Acids Using Topological Indices	885	
S. Kilić and T. Persi: Energy States of Helium-4 Dimer	897	
LJ. Pejov, G. Ivanovski, and V. M. Petruševski: A Quantum Theoretical Basis for Some Spectra – Structure Correlations in Crystalline Hydrates	903	
LJ. Pejov and V. M. Petruševski: An Iterative Perturbation Theory-Based Algorithm for Calculation of Diagonal Force Constants of the v_3 Modes in Quasi-Tetrahedral Systems with Low Anharmonicity	915	
T. P. Živković: Vibrational Isotope Effect of Planar Molecules by the Low Rank Perturbation Method: Deuterated Ethylenes	925	
D. Horvat, Z. Đaković, and T. P. Živković: Self-Consistent Field Low Rank Perturbation Method	945	
D. Vikić-Topić, P. Novak, Z. Meić, J. Plavec, and D. Kovaček: Intrinsic Long Range Deuterium Isotope Effects on ^{13}C NMR Chemical Shifts as a Conformational Probe of Benzene Derivatives	967	

Structural Chemistry

R. Dreos, G. Nardin, L. Randaccio, G. Tauzher, and S. Vuano: The Weak Metal–Water Bond in Diphenylborylated Organo-aquacobaloximes and Rhodoximes Leads to the Formation of an Unusual Dinuclear Rh(III) Complex	231
J. F. Gallagher, E. C. Alyea, and G. Ferguson: Structural Studies of Steric Effects in Phosphine Complexes: Dimers of Bis-{dithiocyanato(1-phenyldibenzophosphole)mercury(II)} Associate with Significant Hg–N and Hg–S Interdimer Interactions	243

- D. Matak-Vinković, M. Bolognesi, A. Battistoni, A. Coda, and K. Djinovic-Carugo:** Crystallographic Study of Mutant Lys120Leu *Xenopus laevis* Cu,Zn Superoxide Dismutase 251
- B. Kojić-Prodić, S. Antolić, M. Kveder, I. Žigrović, J. Kidrič, and Š. Horvat:** Conformational Studies in Solid State and Solution of Protected C-terminal Dipeptide Fragment (Boc-Phe-Pro-NH₂) of Morphiceptin 259
- Z. Popović, D. Matković-Čalogović, J. Hasić, M. Sikirica, and D. Vikić-Topić:** Binding of Mercury(II) by *N*-(2-mercaptopropionyl)glycine. Synthesis, IR and NMR Characterization. Crystal Structure of the 1:2 Solvate of Bis[*N*-(propionyl-2-thiolato)glycine]mercury(II) with 4-Methylpyridine 279
- P. Angerer, E. Tillmanns, and M. Wildner:** Crystal Structure Investigations of Amide Sulfate Tetrahydrates with Divalent Cations 295
- A. Tonejc, A. Tonejc, G. W. Farrants, and S. Hovmöller:** Evidence of Mechanical Alloying in Ball Milled ZrO₂-Y₂O₃ System Based on HRTEM Image Processing Analysis 311
- P. Dapporto, S. Roelens, and P. Rossi:** Crystal and Molecular Structure of the Cyclodimeric Propylene-1,3-phenylenediacetate and of Its Di-*n*-butyltin Dichloride Complex 327
- B. Ya. Kotur and R. Černý:** Disordered Microtwinned (Sc_{1-x})Sc₄Co₆Sn₁₈ (*x* = 0.14) 341
- M. Milanesio, D. Viterbo, S. K. Chatopadhyay, M. Kulshreshtha, and G. Appendino:** Crystal and Molecular Structure of Secoisolariciresinol 351
- A. Prodan, V. Marinković, S. W. Hla, N. Ramšak, F. W. Bostwell, and J. C. Bennett:** Early Stages of Gold and Silver Growth on α-MoTe₂, β-MoTe₂ and WTe₂ 365
- E. W. Ainscough, A. M. Brodie, R. J. Cresswell, J. C. Turnbull, and J. M. Waters:** Phenylcyanamidocupper(I) and Silver(I) Complexes: Synthetic and Structural Studies 377
- G. Štefanić, B. Gržeta, S. Popović, and S. Musić:** *In situ* Phase Analysis of the Thermal Decomposition Products of Zirconium Salts 395
- M. Paljević and M. Tudja:** Selective Oxidation of Zirconium in Zr₂Cu 413

- B. Kozlevčar, N. Lah, I. Leban, I. Turel, P. Šegedin, M. Petrič, F. Pohleven, A. J. P. White, D. J. Williams, and G. Gieser:** Fatty Acid Copper(II) Carboxylates with Nicotinamide - Characterization and Fungicidal Activity. Crystal Structures of Two Heptanoate Forms and Nonanoate 427
- A. Götze, C. Buhrmester, I. Svoboda, and H. Fuess:** Crystal Structures and Phase Transitions of 3-Chloro-2,2-bis(chloromethyl)propionic Acid-1 and 1,3-Dichloro-2,2-dimethylpropane 443
- A. V. Yatsenko, K. A. Paseshnichenko, V. S. Petrosyan, N. S. Yashina, E. V. Grigoriev, and L. A. Aslanov:** Trigonal-bipyramidal Anion $[\text{Ph}_2\text{Cl}_3\text{Sn}]^-$ in the Structure of N -[(Diethylphosphoryl)methyl]piperidinium Diphenyltrichlorostannate (IV) 457
- O. Grupče, G. Jovanovski, B. Kaitner, and P. Naumov:** Structural Investigation of Di- μ -chloro-bis[saccharinatopyridine-mercury(II)] by X-ray Diffraction and FT IR Spectroscopy 465
- B. Udrovic, I. Leban, and P. Šegedin:** The Chaotropically Synthesized Dimolybdenum(II,II) Compound 477
- M. Cindrić, N. Strukan, and V. Vrdoljak:** Synthesis and Characterization of New Molybdenum(VI) Oxalate Complexes. Crystal Structure of Tetramethylammonium Salt of μ -Oxo-di-aquadioxalatotetraoxodimolybdenum(VI) 501
- K. W. Muir, D. G. Morris, and V. Innes:** Crystal Structure of the Phosphinyl-stabilised Ylide $\text{Me}_3\text{NNP}(=\text{O})\text{Ph}_2 \cdot \text{H}_2\text{O}$ 511
- M. C. Burla, C. Giacovazzo, D. Lamba, G. Polidori, and G. Ughetto:** *Ab initio* Direct Phasing in Macromolecular Crystallography: an Application of the Z-test 519
- I. Matijašić, G. Bocelli, C. Rizzoli, and Lj. Tušek-Božić:** Synthesis and Crystal and Molecular Structure of *trans*-[PtCl₂(8-dqmp)₂] (8-dqmp = diethyl 8-quinolylmethylphosphonate) 531
- D. Matak-Vinković, M. Vinković, and M. Dumić:** Chemistry of 1,3-Dioxepins. XIV. Structural Studies of 4,7-Dihydro-(4,7-dihydro-1,3-dioxepin-2-yl)-1,3-dioxepin and Their Metal Complexes 541
- Gy. Argay, L. Fábián, and A. Kálmán:** On the Hydrogen Bonding of Succinimide Derivatives: Crystal Structure of 3-(4-Pyridylmethyl)aminopyrrolidine-2,5-dione 551

- B. Šorgić, Ž. Blažina, and A. Drašner:** The RENi_4Ga ($\text{RE} = \text{Dy}, \text{Ho}, \text{Er}$) Intermetallic Compounds – Crystal Structure and Hydride Properties 567
- V. Dhanaraj, M. G. Williams, Q.-Z. Ye, F. Molina, L. L. Johnson, D. F. Ortwin, A. Pavlovsky, J. R. Rubin, R. W. Skeean, A. D. White, Ch. Humblet, D. J. Hupe, and T. L. Blundell:** X-ray Structure of Gelatinase A Catalytic Domain Complexed with a Hydroxamate Inhibitor 575
- H. Schenk, R. A. J. Driessens, R. de Gelder, K. Goubitz, H. Nieboer, I. E. M. Brüggemann-Rotgans, and P. Diepenhorst:** Elucidation of the Structure of Solanoclepin A, a Natural Hatching Factor of Potato and Tomato Cyst Nematodes, by Single-crystal X-ray Diffraction 593
- B. Kaitner and G. Pavlović:** Hydrogen Bonded Dimer N -(2-hydroxyethyl)-2-oxy-1-naphthalimine and Its Oxo-vanadium(V) Complex 607
- S. Popović and B. Gržeta:** Precipitation and Dissolution Phenomena in Al-Zn Alloys 621
- N. Rajić, I. Arčon, V. Kaučič, and A. Kodre:** A Study of the Mn, Co and Ni Environment in the As-synthesized and Rehydrated-calcined Aluminophosphate with Chabazite-like Topology 645
- B. Šoptrajanov, M. Trpkovska, and Lj. Pejov:** Fourier Transform Infrared Study of Dichlorodioxochromium(VI), Dichlorodioxomolybdenum(VI) and Dichlorodioxotungsten(VI) Complexes with 2,2'-Bipyridine 663
- N. S. Hunter, Th. J. Gleichmann, M. Helliwell, L. Barba, E. Busetto, A. Lausi, H. J. Price, and J. R. Helliwell:** Crystallographic MAD Phasing Strategies Explored Using ELETTRA Sincrotron Mn K-Edge Data to 2.1 Å and Use of CHESS Establishes the Diffraction Resolution Limit as 0.92 Å for the Protein Mn, Ca Concanavalin A 673
- A. F. Marinovich, R. Sh. O'Mahony, J. M. Waters, and T. N. M. Waters:** Schiff Base Complexes of Copper(II) 685

Inorganic Chemistry

- R. Kurpiel-Gorgol and W. Brzyska:** Preparation and Properties of Rare Earth 4-Nitrophthalates 77

- W. Ferenc, B. Bocian, and D. Mazur:** Spectral and Thermal Studies of Light Lanthanide Complexes with 4-Methoxy-3-nitrobenzoic Acid 779

Materials Chemistry

- S. Musić, G. P. Santana, G. Šmit, and V. K. Garg:** ^{57}Fe Mössbauer, FT-IR and TEM Observations of Oxide Phases Precipitated from Concentrated $\text{Fe}(\text{NO}_3)_3$ Solutions 87
- S. Musić, M. Maljković, S. Popović, and R. Trojko:** Formation of Chromia from Amorphous Chromium Hydroxide 789

Organic Chemistry

- V. Kovač, V. Rapić, J. Alagić, and L. Barišić:** Ferrocene Compounds. XXVI. C - and O -Ferrocenylalkylation of Methyl Salicylate 103
- S. Alihodžić and M. Žinić:** Lariat Ethers with Pendant Phenanthridine Units. Synthesis and Complexation of Na- and K-Picrate 803
- B. Žinić, I. Krizmanić, D. Vikić-Topić, and M. Žinić:** 5-Bromo- and 5-Iodo- N -1-sulfonylcystosine Derivatives. Exclusive Formation of Keto-Imino Tautomers 957

Analytical Chemistry

- J. Lovrić, N. Burger, V. Deljac, and Z. Mihalić:** Spectrophotometric Studies of Some Novel Derivatives of Pyridinium Chloride 123
- O. M. Tsivileva:** Correction Factors for Direct Gas Chromatographic Determination of Acrylic Acid in Aqueous Solutions Using Polyethylene Glycol Adipate as Stationary Phase 819
- G. Stanić, B. Jurišić, and D. Brkić:** HPLC Analysis of Esculin and Fraxin in Horse-Chestnut Bark (*Aesculus hippocastanum L.*) 827

Biochemistry

- D. Juretić, A. Jerončić, and D. Zucić:** Sequence Analysis of Membrane Proteins with the Web Server SPLIT 975
- N. Štambuk:** On Circular Coding Properties of Gene and Protein Sequences 999

NOTES

Inorganic Chemistry

- V. M. Petruševski and S. Aleksovska:** Dependence of the Crystal Structure Parameters on the Size of the Structural Units in Some Isomorphous / Isostructural Series 71

Structural Chemistry

- J. Lima-de-Faria:** The Packing Analogues of Sodalite, Tetrahedrite and Related Structures 705

CONFERENCE PAPERS

Physical and Theoretical Chemistry

- S. Nikolić, N. Trinajstić, and S. Ivaniš:** The Connectivity Indices of Regular Graphs 875

AUTHORS REVIEWS

Structural Chemistry

- D. Yu. Pushcharovsky:** New Approaches to the XRD Studies of Complicated Crystal Chemical Phenomena in Minerals 135

- M. Calligaris:** Stereochemical Aspects of Sulfoxides and Metal Sulfoxide Complexes 147

- A. Szytula:** Structural Aspects of Chemical Bonding in RTX Intermetallic Compounds 171

- N. Zabukovec Logar, Lj. Golič, and V. Kaučič:** Recent Developments in Zeolite-like Materials Synthesis and Characterisation 187

- E. Dodson and G. Dodson:** Some Comments on the Crystallography and the Evolution of the Catalytic Structure in Some Serine Hydrolases 209

- B. Bruni, A. Guerri, G. Marcon, L. Messori, and P. Orioli:** Structure and Cytotoxic Properties of Some Selected Gold(III) Complexes 221

PRELIMINARY COMMUNICATIONS

Organic Chemistry

- I. Malnar and O. Kronja: A Case of Concerted Formation of Five
and Six Member Rings; Solvolytic Behavior of 1-Aryl-1-chloro-
4,8,13,17,21-pentamethyl-4,8,12,16,20-docosapentaenes 115
- R. E. Trifonov and V. A. Ostrovskii: An Unusual Formation of
5-Phenyltetrazole in Reaction of Phenylacetylene with Dime-
thylammonium Azide 953

PREFACES

- N. Trinajstić: Editorial I-II
- B. Kaitner and N. Trinajstić: Editorial III
- D. Grdenić: Foreword V-VII
- B. Kamenar – *Curriculum vitae* IX-XI
- T. P. Živković and D. Vikić-Topić: Foreword XV

APPENDICES

- Obituaries A1-A4, A5-A9, A11-A22, A65-A67
- Book Reviews A23-A24, A25-A27, A69
- Meeting of the Croatian Chemical Society (in Croatian) A29-A52
- Statutes of the Croatian Chemical Society (in Croatian) A53-A63
- Instruction to Authors B1-B5
- Announcements and Advertisements C1-C6, C7-C9, C39-C41
- Acknowledgement to Reviewers C11-C13
- Contents and Index of *Croatica Chemica Acta* Vol. 72 C45-C38

